

An analytical condition for the violation of Mermin's inequality by any three qubit state

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Mermin's inequality is the generalization of the Bell-CHSH inequality for three qubit states. The violation of the Mermin inequality guarantees the fact that there exists quantum non-locality either between two or three qubits in a three qubit system. In the absence of an analytical result to this effect, in order to check for the violation of Mermin's inequality one has to perform a numerical optimization procedure for even three qubit pure states. Here we derive an analytical formula for the maximum value of the expectation of the Mermin operator in terms of eigenvalues of symmetric matrices, that gives the maximal violation of the Mermin inequality for all three qubit pure and mixed states.

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I. INTRODUCTION

The impossibility of reproducing the effect of quantum correlations between the outcomes of the distant measurements using local hidden variable theories is known as quantum non-locality. In 1964, Bell constructed an inequality which is satisfied in the absence of non-local correlations between the results of distant measurements [1]. Experimental violation of Bell's inequality confirm the existence of the non-local correlation between the outcome of the measurements. The most well-known form of the Bell inequality is given by Clauser, Horne, Shimony, and Holt (CHSH) and it is known as Bell-CHSH inequality [2]. The Bell-CHSH operator for two qubits is given by $B_{CHSH} = \hat{a} \cdot \vec{\sigma} \otimes (\hat{b} + \hat{b}') \cdot \vec{\sigma} + \hat{a}' \cdot \vec{\sigma} \otimes (\hat{b} - \hat{b}') \cdot \vec{\sigma}$, where $\hat{a}, \hat{a}', \hat{b}, \hat{b}'$ are unit vectors in R^3 . The Bell-CHSH inequality is then given by $|\langle B_{CHSH} \rangle_\rho| \leq 2$, where ρ denotes any two qubit pure or mixed state. This inequality is violated by any two qubit pure entangled state, but on the contrary not all two qubit mixed entangled states violate the Bell-CHSH inequality.

Foundational interest in nonlocality is bolstered through its connection with information theoretic tasks such as teleportation [3]. Quantum nonlocality finds applications in several information theoretic protocols such as device independent quantum key generation [4], quantum state estimation [5], and communication complexity [6], where the amount of violation of the Bell-CHSH inequality is important. In order to obtain the maximal violation of the Bell-CHSH inequality, one has to calculate the expectation of the Bell-CHSH operator by maximizing over all measurements of spin in the directions $\hat{a}, \hat{a}', \hat{b}, \hat{b}'$. Therefore, the problem of maximal violation of the Bell-CHSH inequality reduces to an optimization problem. The optimization problem for the two qubit system was analytically solved by Horodecki [15] by expressing the value of $\langle B_{max} \rangle_\rho$ in terms of the eigenvalues of the symmetric matrix $T_\rho^T T_\rho$, where T_ρ is the correlation matrix of the state ρ . Therefore,

the maximal violation of the Bell-CHSH inequality depends on the eigenvalues of the symmetric matrix $T_\rho^T T_\rho$.

Like two qubit non-locality, non-locality for three qubit systems has also been studied using various approaches. A generalized form of the Bell-CHSH inequality was obtained for three qubits called Mermin's inequality [7] which can be violated by not only genuine entangled three qubit states but also by biseparable states. On the other hand, all genuine entangled three qubit states violate the Svetlichny inequality [8]. There has been quite a bit of recent interest in studying the nonlocality of tripartite systems. A notable direction in this context is the so-called 'superactivation of nonlocality' [9] which has been investigated also for the case of three qubits [10, 11]. The relation of nonlocality with quantum uncertainty has been exhibited for tripartite systems using fine-graining [12], in the context of biased [13] and unbiased quantum games. The security of quantum cryptography is connected with quantum nonlocality [14], that is especially relevant in the context of device independent quantum key distribution.

Violation of the Mermin inequality has been computed for several three qubit states such as GHZ and W-states earlier [16–19]. In order to find the maximum violation of the Mermin inequality for three qubit states one has to tackle the optimization problem numerically because there does not exist any analytical formula for even pure three qubit states. Motivated by the work of Horodecki [15] in the context of two qubit systems, in the present work we perform the optimization problem involved in the Mermin inequality analytically and obtain a formula for the maximal value of the expectation of the Mermin operator in terms of the eigenvalues of symmetric matrices, that gives the maximal violation of the Mermin inequality not only for pure states but also for mixed states. The plan of this paper is as follows. In section-II, we solve the optimization problem analytically and obtain the maximum value of the expectation of the Mermin operator in terms of eigenvalues. In section-III, we provide a few examples where the magnitude of the Mermin operator is calculated using our derived formula for pure and mixed states. Certain concluding remarks are presented in section-IV.

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II. MAXIMUM VALUE OF THE EXPECTATION OF THE MERMIN OPERATOR IN TERMS OF EIGENVALUES

Let B_M be the Mermin operator defined as [19]

$$B_M = \hat{a}_1 \cdot \vec{\sigma} \otimes \hat{a}_2 \cdot \vec{\sigma} \otimes \hat{a}_3 \cdot \vec{\sigma} - \hat{a}_1 \cdot \vec{\sigma} \otimes \hat{b}_2 \cdot \vec{\sigma} \otimes \hat{b}_3 \cdot \vec{\sigma} \\ - \hat{b}_1 \cdot \vec{\sigma} \otimes \hat{a}_2 \cdot \vec{\sigma} \otimes \hat{b}_3 \cdot \vec{\sigma} - \hat{b}_1 \cdot \vec{\sigma} \otimes \hat{b}_2 \cdot \vec{\sigma} \otimes \hat{a}_3 \cdot \vec{\sigma} \quad (1)$$

where \hat{a}_j and \hat{b}_j ($j=1,2,3$) are unit vectors in R^3 , and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of the Pauli matrices.

For any three qubit state ρ , the Mermin inequality is

$$\langle B_M \rangle_\rho \leq 2 \quad (2)$$

where

$$\rho = \frac{1}{8} [I \otimes I \otimes I + \vec{l} \cdot \vec{\sigma} \otimes I \otimes I + I \otimes \vec{m} \cdot \vec{\sigma} \otimes I \\ + I \otimes I \otimes \vec{n} \cdot \vec{\sigma} + \vec{u} \cdot \vec{\sigma} \otimes \vec{v} \cdot \vec{\sigma} \otimes I + \vec{u} \cdot \vec{\sigma} \otimes I \otimes \vec{w} \cdot \vec{\sigma} \\ + I \otimes \vec{v} \cdot \vec{\sigma} \otimes \vec{w} \cdot \vec{\sigma} + \sum_{i,j,k=x,y,z} t_{ijk} \sigma_i \otimes \sigma_j \otimes \sigma_k] \quad (3)$$

with

$$l_i = \text{Tr}(\rho(\sigma_i \otimes I \otimes I)), m_i = \text{Tr}(\rho(I \otimes \sigma_i \otimes I)), \\ n_i = \text{Tr}(\rho(I \otimes I \otimes \sigma_i)), (i = x, y, z) \quad (4)$$

$$u_i v_i = \text{Tr}(\rho(\sigma_i \otimes \sigma_i \otimes I)), u_i w_i = \text{Tr}(\rho(\sigma_i \otimes I \otimes \sigma_i)), \\ v_i w_i = \text{Tr}(\rho(I \otimes \sigma_i \otimes \sigma_i)), (i = x, y, z) \quad (5)$$

$$t_{ijk} = \text{Tr}(\rho(\sigma_i \otimes \sigma_j \otimes \sigma_k)), (i, j, k = x, y, z) \quad (6)$$

We will now derive the necessary and sufficient condition which tells us that when a three-qubit state ρ violates Mermin's inequality. The expectation value of the Mermin operator with respect to the state ρ given by (3) is

$$\langle B_M \rangle_\rho = \text{Tr}(B_M \rho) \\ = \sum_{i,j,k=x,y,z} a_{1i} a_{2j} a_{3k} t_{ijk} \\ - \sum_{i,j,k=x,y,z} a_{1i} b_{2j} b_{3k} t_{ijk} \\ - \sum_{i,j,k=x,y,z} b_{1i} a_{2j} b_{3k} t_{ijk} \\ - \sum_{i,j,k=x,y,z} b_{1i} b_{2j} a_{3k} t_{ijk} \\ = (\hat{a}_1, \hat{a}_3^T \vec{T} \hat{a}_2) - (\hat{a}_1, \hat{b}_3^T \vec{T} \hat{b}_2) \\ - (\hat{b}_1, \hat{b}_3^T \vec{T} \hat{a}_2) - (\hat{b}_1, \hat{a}_3^T \vec{T} \hat{b}_2) \quad (7)$$

where $\hat{a}_s = (a_{sx}, a_{sy}, a_{sz})$ and $\hat{b}_s = (b_{sx}, b_{sy}, b_{sz})$, ($s=1,2,3$) and (\vec{x}, \vec{y}) denotes the inner product of two vectors \vec{x} and \vec{y} and is defined as $(\vec{x}, \vec{y}) = \|\vec{x}\| \|\vec{y}\| \cos \theta$, θ being the angle between \vec{x} and \vec{y} . The superscript T refers to trans-

pose, and $\vec{T} = (T_x, T_y, T_z)$; $T_x = \begin{pmatrix} t_{xxx} & t_{xyx} & t_{xzx} \\ t_{xxy} & t_{xyy} & t_{xzy} \\ t_{xxz} & t_{xyz} & t_{xzz} \end{pmatrix}$,

$$T_y = \begin{pmatrix} t_{yyx} & t_{yyy} & t_{yyz} \\ t_{yxy} & t_{yyy} & t_{yzy} \\ t_{yxz} & t_{yyz} & t_{yzz} \end{pmatrix}, T_z = \begin{pmatrix} t_{zxx} & t_{zyx} & t_{zzx} \\ t_{zxy} & t_{zyy} & t_{zzy} \\ t_{zxx} & t_{zyz} & t_{zzz} \end{pmatrix}$$

Theorem-1: If the symmetric matrices $T_x^T T_x$, $T_y^T T_y$ and $T_z^T T_z$ have unique largest eigenvalues λ_x^{max} , λ_y^{max} and λ_z^{max} respectively, then Mermin's inequality is violated if

$$\langle B_M^{max} \rangle_\rho = \max_{B_M} \text{Tr}(B_M \rho) \\ = \max\{2\sqrt{\lambda_x^{max}}, 2\sqrt{\lambda_y^{max}}, 2\sqrt{\lambda_z^{max}}\} \\ > 2 \quad (8)$$

Proof: In the expression for $\langle B_M \rangle_\rho$ given by Eq.(7), we first simplify the vectors $\hat{a}_3^T \vec{T} \hat{a}_2$, $\hat{b}_3^T \vec{T} \hat{b}_2$, $\hat{b}_3^T \vec{T} \hat{a}_2$, $\hat{a}_3^T \vec{T} \hat{b}_2$. We choose the vectors \hat{a}_2 , \hat{a}_3 , \hat{b}_2 and \hat{b}_3 in such a way that they maximize the quantity $\langle B_M \rangle_\rho$ over all the operators B_M . Let us proceed by considering the following cases sequentially:

Case-I: In this case we choose the vectors in such a way that the maximized expectation value of the Mermin operator is given by $\langle B_M^{(1)} \rangle_\rho = 2\sqrt{\lambda_x^{max}}$.

(i) The vector $\hat{a}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\hat{a}_3^T \vec{T} \hat{a}_2 = ((\hat{a}_3, T_x \hat{a}_2), (\hat{a}_3, T_y \hat{a}_2), (\hat{a}_3, T_z \hat{a}_2)) \\ = (\|\hat{a}_3^{max}\| \|T_x \hat{a}_2\|, 0, 0) \quad (9)$$

where \hat{a}_3^{max} is a unit vector along $T_x \hat{a}_2$ and perpendicular to $T_y \hat{a}_2$ and $T_z \hat{a}_2$. Since \hat{a}_3^{max} is a unit vector, $\|\hat{a}_3^{max}\| = 1$. Again, $\|T_x \hat{a}_2\|^2 = (T_x \hat{a}_2, T_x \hat{a}_2) = (\hat{a}_2, T_x^T T_x \hat{a}_2)$. If λ_x^{max} is the largest eigenvalue of the symmetric matrix $T_x^T T_x$ and \hat{a}_2^{max} is the corresponding unit vector, then $\|T_x \hat{a}_2\|^2 = (\hat{a}_2, T_x^T T_x \hat{a}_2) = (\hat{a}_2, \lambda_x^{max} \hat{a}_2^{max})$. If \hat{a}_2 is the unit vector along \hat{a}_2^{max} , then $\|T_x \hat{a}_2\|^2 = \lambda_x^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{a}_2 = (\sqrt{\lambda_x^{max}}, 0, 0) \quad (10)$$

(ii) The vector $\hat{a}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\hat{a}_3^T \vec{T} \hat{b}_2 = ((\hat{a}_3, T_x \hat{b}_2), (\hat{a}_3, T_y \hat{b}_2), (\hat{a}_3, T_z \hat{b}_2)) \\ = (0, -\|\hat{a}_3^{min}\| \|T_y \hat{b}_2\|, 0) \quad (11)$$

where \hat{a}_3^{min} is the unit vector antiparallel to $T_y \hat{b}_2$ and perpendicular to $T_x \hat{b}_2$ and $T_z \hat{b}_2$. Since \hat{a}_3^{min} is a unit vector, $\|\hat{a}_3^{min}\| = 1$. Again, $\|T_y \hat{b}_2\|^2 = (T_y \hat{b}_2, T_y \hat{b}_2) = (\hat{b}_2, T_y^T T_y \hat{b}_2)$. If λ_y^{max} is the largest eigenvalue of the symmetric matrix $T_y^T T_y$ and \hat{b}_2^{max} is the corresponding unit vector, then $\|T_y \hat{b}_2\|^2 = (\hat{b}_2, T_y^T T_y \hat{b}_2) = (\hat{b}_2, \lambda_y^{max} \hat{b}_2^{max})$. If \hat{b}_2 is the unit vector along \hat{b}_2^{max} , then $\|T_y \hat{b}_2\|^2 = \lambda_y^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{b}_2 = (0, -\sqrt{\lambda_y^{max}}, 0) \quad (12)$$

(iii) The vector $\hat{b}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\hat{b}_3^T \vec{T} \hat{b}_2 = ((\hat{b}_3, T_x \hat{b}_2), (\hat{b}_3, T_y \hat{b}_2), (\hat{b}_3, T_z \hat{b}_2)) \\ = (0, -\|\hat{b}_3^{min}\| \|T_y \hat{b}_2\|, 0) \\ = (0, -\sqrt{\lambda_y^{max}}, 0) \quad (13)$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_y \hat{b}_2$ and perpendicular to $T_x \hat{b}_2$ and $T_z \hat{b}_2$. Since \hat{b}_3^{min} is a unit vector, $\|\hat{b}_3^{min}\| = 1$.

(iv) The vector $\hat{b}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned} \hat{b}_3^T \vec{T} \hat{a}_2 &= ((\hat{b}_3, T_x \hat{a}_2), (\hat{b}_3, T_y \hat{a}_2), (\hat{b}_3, T_z \hat{a}_2)) \\ &= (\|\hat{b}_3^{max}\| \|T_x \hat{a}_2\|, 0, 0) = (\sqrt{\lambda_x^{max}}, 0, 0) \end{aligned} \quad (14)$$

where \hat{b}_3^{max} is the unit vector along $T_x \hat{a}_2$ and perpendicular to $T_y \hat{a}_2$ and $T_z \hat{a}_2$.

From (7),(10),(12),(13),(14), we have

$$\begin{aligned} \langle B_M^{(1)} \rangle_\rho &= \max_{\hat{a}_1, \hat{b}_1} [(\hat{a}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) \\ &+ (\hat{a}_1, (0, \sqrt{\lambda_y^{max}}, 0)) - (\hat{b}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) \\ &+ (\hat{b}_1, (0, \sqrt{\lambda_y^{max}}, 0))] \\ &= \|\hat{a}_1^{max}\| \|(\sqrt{\lambda_x^{max}}, 0, 0)\| \\ &+ \|\hat{b}_1^{max}\| \|(\sqrt{\lambda_x^{max}}, 0, 0)\| \\ &= 2\sqrt{\lambda_x^{max}} \end{aligned} \quad (15)$$

\hat{a}_1^{max} is the unit vector parallel to $(\sqrt{\lambda_x^{max}}, 0, 0)$ and perpendicular to $(0, \sqrt{\lambda_y^{max}}, 0)$; \hat{b}_1^{max} is the unit vectors antiparallel to $(\sqrt{\lambda_x^{max}}, 0, 0)$ and perpendicular to $(0, \sqrt{\lambda_y^{max}}, 0)$.

Case-II: In this case we choose the vectors in such a way that the maximized expectation value of the Mermin operator is given by $\langle B_M^{(2)} \rangle_\rho = 2\sqrt{\lambda_y^{max}}$.

(i) The vector $\hat{a}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned} \hat{a}_3^T \vec{T} \hat{a}_2 &= ((\hat{a}_3, T_x \hat{a}_2), (\hat{a}_3, T_y \hat{a}_2), (\hat{a}_3, T_z \hat{a}_2)) \\ &= (0, \|\hat{a}_3^{max}\| \|T_y \hat{a}_2\|, 0) \end{aligned} \quad (16)$$

where \hat{a}_3^{max} is the unit vector along $T_y \hat{a}_2$ and perpendicular to $T_x \hat{a}_2$ and $T_z \hat{a}_2$. Repeating the steps of Case-I, we find

$$\hat{a}_3^T \vec{T} \hat{a}_2 = (0, \sqrt{\lambda_y^{max}}, 0) \quad (17)$$

(ii) Similarly, we obtain

$$\hat{a}_3^T \vec{T} \hat{b}_2 = (-\sqrt{\lambda_x^{max}}, 0, 0) \quad (18)$$

, (iii) and

$$\begin{aligned} \hat{b}_3^T \vec{T} \hat{b}_2 &= ((\hat{b}_3, T_x \hat{b}_2), (\hat{b}_3, T_y \hat{b}_2), (\hat{b}_3, T_z \hat{b}_2)) \\ &= (-\|\hat{b}_3^{min}\| \|T_x \hat{b}_2\|, 0, 0) \\ &= (-\sqrt{\lambda_x^{max}}, 0, 0) \end{aligned} \quad (19)$$

, (iv) and

$$\begin{aligned} \hat{b}_3^T \vec{T} \hat{a}_2 &= ((\hat{b}_3, T_x \hat{a}_2), (\hat{b}_3, T_y \hat{a}_2), (\hat{b}_3, T_z \hat{a}_2)) \\ &= (0, \|\hat{b}_3^{max}\| \|T_y \hat{a}_2\|, 0) = (0, \sqrt{\lambda_y^{max}}, 0) \end{aligned} \quad (20)$$

where \hat{b}_3^{max} is the unit vector along $T_y \hat{a}_2$ and perpendicular to $T_x \hat{a}_2$ and $T_z \hat{a}_2$.

Now, from (7),(17),(18),(19),(20), we have

$$\begin{aligned} \langle B_M^{(2)} \rangle_\rho &= \max_{\hat{a}_1, \hat{b}_1} [(\hat{a}_1, (0, \sqrt{\lambda_y^{max}}, 0)) \\ &+ (\hat{a}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) - (\hat{b}_1, (0, \sqrt{\lambda_y^{max}}, 0)) \\ &+ (\hat{b}_1, (\sqrt{\lambda_x^{max}}, 0, 0))] \\ &= \|\hat{a}_1^{max}\| \|(0, \sqrt{\lambda_y^{max}}, 0)\| \\ &+ \|\hat{b}_1^{max}\| \|(0, \sqrt{\lambda_y^{max}}, 0)\| \\ &= 2\sqrt{\lambda_y^{max}} \end{aligned} \quad (21)$$

where \hat{a}_1^{max} is the unit vector parallel to $(0, \sqrt{\lambda_y^{max}}, 0)$ and perpendicular to $(\sqrt{\lambda_x^{max}}, 0, 0)$; \hat{b}_1^{max} is the unit vectors antiparallel to $(0, \sqrt{\lambda_y^{max}}, 0)$ and perpendicular to $(\sqrt{\lambda_x^{max}}, 0, 0)$.

Case-III: In this case we choose the vectors in such a way that the maximized expectation value of the Mermin operator is given by $\langle B_M^{(3)} \rangle_\rho = 2\sqrt{\lambda_z^{max}}$.

Again, repeating the above steps, we find (i) The vector $\hat{a}_3^T \vec{T} \hat{a}_2$ can be simplified to

$$\hat{a}_3^T \vec{T} \hat{a}_2 = (0, 0, \sqrt{\lambda_z^{max}}) \quad (22)$$

, (ii) The vector $\hat{a}_3^T \vec{T} \hat{b}_2$ can be simplified to

$$\hat{a}_3^T \vec{T} \hat{b}_2 = (-\sqrt{\lambda_x^{max}}, 0, 0) \quad (23)$$

(iii) The vector $\hat{b}_3^T \vec{T} \hat{b}_2$ can be simplified to

$$\begin{aligned} \hat{b}_3^T \vec{T} \hat{b}_2 &= ((\hat{b}_3, T_x \hat{b}_2), (\hat{b}_3, T_y \hat{b}_2), (\hat{b}_3, T_z \hat{b}_2)) \\ &= (-\|\hat{b}_3^{min}\| \|T_x \hat{b}_2\|, 0, 0) \\ &= (-\sqrt{\lambda_x^{max}}, 0, 0) \end{aligned} \quad (24)$$

(iv) The vector $\hat{b}_3^T \vec{T} \hat{a}_2$ can be simplified to

$$\begin{aligned} \hat{b}_3^T \vec{T} \hat{a}_2 &= ((\hat{b}_3, T_x \hat{a}_2), (\hat{b}_3, T_y \hat{a}_2), (\hat{b}_3, T_z \hat{a}_2)) \\ &= (0, 0, \|\hat{b}_3^{max}\| \|T_z \hat{a}_2\|) = (0, 0, \sqrt{\lambda_z^{max}}) \end{aligned} \quad (25)$$

Now, from (7),(22),(23),(24),(25), we have

$$\begin{aligned} \langle B_M^{(3)} \rangle_\rho &= \max_{\hat{a}_1, \hat{b}_1} [(\hat{a}_1, (0, 0, \sqrt{\lambda_z^{max}})) \\ &+ (\hat{a}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) - (\hat{b}_1, (0, 0, \sqrt{\lambda_z^{max}})) \\ &+ (\hat{b}_1, (\sqrt{\lambda_x^{max}}, 0, 0))] \\ &= \|\hat{a}_1^{max}\| \|(0, 0, \sqrt{\lambda_z^{max}})\| \\ &+ \|\hat{b}_1^{max}\| \|(0, 0, \sqrt{\lambda_z^{max}})\| \\ &= 2\sqrt{\lambda_z^{max}} \end{aligned} \quad (26)$$

where, \hat{a}_1^{max} is the unit vector parallel to $(0, 0, \sqrt{\lambda_z^{max}})$ and perpendicular to $(\sqrt{\lambda_x^{max}}, 0, 0)$; \hat{b}_1^{max} is the unit vectors antiparallel to $(0, 0, \sqrt{\lambda_z^{max}})$ and perpendicular to $(\sqrt{\lambda_x^{max}}, 0, 0)$.

Thus finally, the maximum expectation value of the Mermin operator with respect to the state ρ is given by

$$\begin{aligned}\langle B_M^{max} \rangle_\rho &= \max\{\langle B_M^{(1)} \rangle_\rho, \langle B_M^{(2)} \rangle_\rho, \langle B_M^{(3)} \rangle_\rho\} \\ &= \max\{2\sqrt{\lambda_x^{max}}, 2\sqrt{\lambda_y^{max}}, 2\sqrt{\lambda_z^{max}}\}\end{aligned}\quad (27)$$

The Mermin inequality is violated if

$$\begin{aligned}\langle B_M^{max} \rangle_\rho &> 2 \\ \Rightarrow \max\{2\sqrt{\lambda_x^{max}}, 2\sqrt{\lambda_y^{max}}, 2\sqrt{\lambda_z^{max}}\} &> 2 \\ \Rightarrow \max\{\sqrt{\lambda_x^{max}}, \sqrt{\lambda_y^{max}}, \sqrt{\lambda_z^{max}}\} &> 1\end{aligned}\quad (28)$$

Hence, proved.

Theorem-2: If the symmetric matrices $T_x^T T_x, T_y^T T_y$ and $T_z^T T_z$ have two equal largest eigenvalue $\lambda_x^{max}, \lambda_y^{max}$ and λ_z^{max} respectively then Mermin's inequality is violated if

$$\begin{aligned}\langle B_M^{max} \rangle_\rho &= \max_{B_M} \text{Tr}(B_M \rho) \\ &= \max\{4\sqrt{\lambda_x^{max}}, 4\sqrt{\lambda_y^{max}}, 4\sqrt{\lambda_z^{max}}\} \\ &> 2\end{aligned}\quad (29)$$

Proof: In the expression for $\langle B_M \rangle_\rho$ given by Eq. (7), we first simplify the vectors $\hat{a}_3^T \vec{T} \hat{a}_2, \hat{b}_3^T \vec{T} \hat{b}_2, \hat{b}_3^T \vec{T} \hat{a}_2, \hat{a}_3^T \vec{T} \hat{b}_2$. We again consider the following cases:

Case-I: We consider the symmetric matrix $T_x^T T_x$ which has two equal largest eigenvalues λ_x^{max} and choose the unit vectors in such a way that it maximizes the expectation value of the Mermin operator given by $\langle B_M^{(4)} \rangle_\rho = 4\sqrt{\lambda_x^{max}}$.

(i) The vector $\hat{a}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned}\hat{a}_3^T \vec{T} \hat{a}_2 &= ((\hat{a}_3, T_x \hat{a}_2), (\hat{a}_3, T_y \hat{a}_2), (\hat{a}_3, T_z \hat{a}_2)) \\ &= (\|\hat{a}_3^{max}\| \|T_x \hat{a}_2\|, 0, 0)\end{aligned}\quad (30)$$

where \hat{a}_3^{max} is the unit vector along $T_x \hat{a}_2$ and perpendicular to $T_y \hat{a}_2$ and $T_z \hat{a}_2$. Since \hat{a}_3^{max} is a unit vector, $\|\hat{a}_3^{max}\| = 1$. Again, $\|T_x \hat{a}_2\|^2 = (T_x \hat{a}_2, T_x \hat{a}_2) = (\hat{a}_2, T_x^T T_x \hat{a}_2)$. If λ_x^{max} is the largest eigenvalue of the symmetric matrix $T_x^T T_x$ and \hat{a}_2^{max} is the corresponding unit eigenvector then $\|T_x \hat{a}_2\|^2 = (\hat{a}_2, T_x^T T_x \hat{a}_2) = (\hat{a}_2, \lambda_x^{max} \hat{a}_2^{max})$. If \hat{a}_2 is the unit vector along \hat{a}_2^{max} then $\|T_x \hat{a}_2\|^2 = \lambda_x^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{a}_2 = (\sqrt{\lambda_x^{max}}, 0, 0)\quad (31)$$

(ii) The vector $\hat{a}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned}\hat{a}_3^T \vec{T} \hat{b}_2 &= ((\hat{a}_3, T_x \hat{b}_2), (\hat{a}_3, T_y \hat{b}_2), (\hat{a}_3, T_z \hat{b}_2)) \\ &= (-\|\hat{a}_3^{min}\| \|T_x \hat{b}_2\|, 0, 0)\end{aligned}\quad (32)$$

where \hat{a}_3^{min} is the unit vector antiparallel to $T_x \hat{b}_2$ and perpendicular to $T_y \hat{b}_2$ and $T_z \hat{b}_2$. Since \hat{a}_3^{min} is the unit vector so $\|\hat{a}_3^{min}\| = 1$. Again, $\|T_x \hat{b}_2\|^2 = (T_x \hat{b}_2, T_x \hat{b}_2) = (\hat{b}_2, T_x^T T_x \hat{b}_2)$. Since the matrix $T_x^T T_x$ has two equal largest eigenvalues λ_x^{max} , so \hat{b}_2^{max} is another corresponding unit eigenvector. Then $\|T_x \hat{b}_2\|^2 = (\hat{b}_2, T_x^T T_x \hat{b}_2) =$

$(\hat{b}_2, \lambda_x^{max} \hat{b}_2^{max})$. If \hat{b}_2 is the unit vector along \hat{b}_2^{max} then $\|T_x \hat{b}_2\|^2 = \lambda_x^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{b}_2 = (-\sqrt{\lambda_x^{max}}, 0, 0)\quad (33)$$

(iii) The vector $\hat{b}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned}\hat{b}_3^T \vec{T} \hat{b}_2 &= ((\hat{b}_3, T_x \hat{b}_2), (\hat{b}_3, T_y \hat{b}_2), (\hat{b}_3, T_z \hat{b}_2)) \\ &= (-\|\hat{b}_3^{min}\| \|T_x \hat{b}_2\|, 0, 0) \\ &= (-\sqrt{\lambda_x^{max}}, 0, 0)\end{aligned}\quad (34)$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_x \hat{b}_2$ and perpendicular to $T_y \hat{b}_2$ and $T_z \hat{b}_2$.

(iv) The vector $\hat{b}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned}\hat{b}_3^T \vec{T} \hat{a}_2 &= ((\hat{b}_3, T_x \hat{a}_2), (\hat{b}_3, T_y \hat{a}_2), (\hat{b}_3, T_z \hat{a}_2)) \\ &= (-\|\hat{b}_3^{min}\| \|T_x \hat{a}_2\|, 0, 0) \\ &= (-\sqrt{\lambda_x^{max}}, 0, 0)\end{aligned}\quad (35)$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_x \hat{a}_2$ and perpendicular to $T_y \hat{a}_2$ and $T_z \hat{a}_2$.

From (7),(31),(33),(34),(35), we have

$$\begin{aligned}\langle B_M^{(4)} \rangle_\rho &= \max_{\hat{a}_1, \hat{b}_1} [(\hat{a}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) \\ &+ (\hat{a}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) + (\hat{b}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) \\ &+ (\hat{b}_1, (\sqrt{\lambda_x^{max}}, 0, 0))] \\ &= 2\|\hat{a}_1^{max}\| \|(\sqrt{\lambda_x^{max}}, 0, 0)\| \\ &+ 2\|\hat{b}_1^{max}\| \|(\sqrt{\lambda_x^{max}}, 0, 0)\| \\ &= 4\sqrt{\lambda_x^{max}}\end{aligned}\quad (36)$$

where \hat{a}_1^{max} and \hat{b}_1^{max} is the unit vector along $(\sqrt{\lambda_x^{max}}, 0, 0)$.

Case-II: Here we consider the symmetric matrix $T_y^T T_y$ which has two equal largest eigenvalues λ_y^{max} and choose the unit vectors in such a way that it maximizes the expectation value of the Mermin operator given by $\langle B_M^{(5)} \rangle_\rho = 4\sqrt{\lambda_y^{max}}$.

(i) The vector $\hat{a}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned}\hat{a}_3^T \vec{T} \hat{a}_2 &= ((\hat{a}_3, T_x \hat{a}_2), (\hat{a}_3, T_y \hat{a}_2), (\hat{a}_3, T_z \hat{a}_2)) \\ &= (0, \|\hat{a}_3^{max}\| \|T_y \hat{a}_2\|, 0)\end{aligned}\quad (37)$$

where \hat{a}_3^{max} is the unit vector along $T_y \hat{a}_2$ and perpendicular to $T_x \hat{a}_2$ and $T_z \hat{a}_2$. Since \hat{a}_3^{max} is a unit vector, $\|\hat{a}_3^{max}\| = 1$. Again, $\|T_y \hat{a}_2\|^2 = (T_y \hat{a}_2, T_y \hat{a}_2) = (\hat{a}_2, T_y^T T_y \hat{a}_2)$. If λ_y^{max} is the largest eigenvalue of the symmetric matrix $T_y^T T_y$ and \hat{a}_2^{max} is the corresponding unit eigenvector then $\|T_y \hat{a}_2\|^2 = (\hat{a}_2, T_y^T T_y \hat{a}_2) = (\hat{a}_2, \lambda_y^{max} \hat{a}_2^{max})$. If \hat{a}_2 is the unit vector along \hat{a}_2^{max} then $\|T_y \hat{a}_2\|^2 = \lambda_y^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{a}_2 = (0, \sqrt{\lambda_y^{max}}, 0)\quad (38)$$

(ii) The vector $\hat{a}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned}\hat{a}_3^T \vec{T} \hat{b}_2 &= ((\hat{a}_3, T_x \hat{b}_2), (\hat{a}_3, T_y \hat{b}_2), (\hat{a}_3, T_z \hat{b}_2)) \\ &= (0, -\|\hat{a}_3^{min}\| \|T_y \hat{b}_2\|, 0)\end{aligned}\quad (39)$$

where \hat{a}_3^{min} is the unit vector antiparallel to $T_y \hat{b}_2$ and perpendicular to $T_x \hat{b}_2$ and $T_z \hat{b}_2$. Since \hat{a}_3^{min} is a unit vector so $\|\hat{a}_3^{min}\| = 1$. Again, $\|T_y \hat{b}_2\|^2 = (T_y \hat{b}_2, T_y \hat{b}_2) = (\hat{b}_2, T_y^T T_y \hat{b}_2)$. Since the matrix $T_y^T T_y$ has two equal largest eigenvalues λ_y^{max} , so let us consider \hat{b}_2^{max} be another corresponding unit eigenvector. Then $\|T_y \hat{b}_2\|^2 = (\hat{b}_2, T_y^T T_y \hat{b}_2) = (\hat{b}_2, \lambda_y^{max} \hat{b}_2^{max})$. If \hat{b}_2 is the unit vector along \hat{b}_2^{max} , then $\|T_y \hat{b}_2\|^2 = \lambda_y^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{b}_2 = (0, -\sqrt{\lambda_y^{max}}, 0) \quad (40)$$

(iii) The vector $\hat{b}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned}\hat{b}_3^T \vec{T} \hat{b}_2 &= ((\hat{b}_3, T_x \hat{b}_2), (\hat{b}_3, T_y \hat{b}_2), (\hat{b}_3, T_z \hat{b}_2)) \\ &= (0, -\|\hat{b}_3^{min}\| \|T_y \hat{b}_2\|, 0) \\ &= (0, -\sqrt{\lambda_y^{max}}, 0)\end{aligned}\quad (41)$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_y \hat{b}_2$ and perpendicular to $T_x \hat{b}_2$ and $T_z \hat{b}_2$.

(iv) The vector $\hat{b}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned}\hat{b}_3^T \vec{T} \hat{a}_2 &= ((\hat{b}_3, T_x \hat{a}_2), (\hat{b}_3, T_y \hat{a}_2), (\hat{b}_3, T_z \hat{a}_2)) \\ &= (0, -\|\hat{b}_3^{min}\| \|T_y \hat{a}_2\|, 0) \\ &= (0, -\sqrt{\lambda_y^{max}}, 0)\end{aligned}\quad (42)$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_y \hat{a}_2$ and perpendicular to $T_x \hat{a}_2$ and $T_z \hat{a}_2$.

From (7),(38),(40),(41),(42), we have

$$\begin{aligned}\langle B_M^{(5)} \rangle_\rho &= \max_{\hat{a}_1, \hat{b}_1} [(\hat{a}_1, (0, \sqrt{\lambda_y^{max}}, 0)) \\ &\quad + (\hat{a}_1, (0, \sqrt{\lambda_y^{max}}, 0)) + (\hat{b}_1, (0, \sqrt{\lambda_y^{max}}, 0)) \\ &\quad + (\hat{b}_1, (0, \sqrt{\lambda_y^{max}}, 0))] \\ &= 2\|\hat{a}_1^{max}\| \|(0, \sqrt{\lambda_y^{max}}, 0)\| \\ &\quad + 2\|\hat{b}_1^{max}\| \|(0, \sqrt{\lambda_y^{max}}, 0)\| \\ &= 4\sqrt{\lambda_y^{max}}\end{aligned}\quad (43)$$

where \hat{a}_1^{max} and \hat{b}_1^{max} is the unit vector along $(0, \sqrt{\lambda_y^{max}}, 0)$.

Case-III: Here we consider the symmetric matrix $T_y^T T_y$ which has two equal largest eigenvalues λ_y^{max} and choose the unit vectors in such a way that it maximizes the expectation

value of the Mermin operator, given by $\langle B_M^{(6)} \rangle_\rho = 4\sqrt{\lambda_z^{max}}$.

(i) The vector $\hat{a}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned}\hat{a}_3^T \vec{T} \hat{a}_2 &= ((\hat{a}_3, T_x \hat{a}_2), (\hat{a}_3, T_y \hat{a}_2), (\hat{a}_3, T_z \hat{a}_2)) \\ &= (0, 0, \|\hat{a}_3^{max}\| \|T_z \hat{a}_2\|)\end{aligned}\quad (44)$$

where \hat{a}_3^{max} is the unit vector along $T_z \hat{a}_2$ and perpendicular to $T_x \hat{a}_2$ and $T_y \hat{a}_2$. Since \hat{a}_3^{max} is a unit vector, $\|\hat{a}_3^{max}\| = 1$. Again, $\|T_z \hat{a}_2\|^2 = (T_z \hat{a}_2, T_z \hat{a}_2) = (\hat{a}_2, T_z^T T_z \hat{a}_2)$. If λ_z^{max} is the largest eigenvalue of the symmetric matrix $T_z^T T_z$ and \hat{a}_2^{max} is the corresponding unit eigenvector, then $\|T_z \hat{a}_2\|^2 = (\hat{a}_2, T_z^T T_z \hat{a}_2) = (\hat{a}_2, \lambda_z^{max} \hat{a}_2^{max})$. If \hat{a}_2 is the unit vector along \hat{a}_2^{max} , then $\|T_z \hat{a}_2\|^2 = \lambda_z^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{a}_2 = (0, 0, \sqrt{\lambda_z^{max}}) \quad (45)$$

(ii) The vector $\hat{a}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned}\hat{a}_3^T \vec{T} \hat{b}_2 &= ((\hat{a}_3, T_x \hat{b}_2), (\hat{a}_3, T_y \hat{b}_2), (\hat{a}_3, T_z \hat{b}_2)) \\ &= (0, 0, -\|\hat{a}_3^{min}\| \|T_z \hat{b}_2\|)\end{aligned}\quad (46)$$

where \hat{a}_3^{min} is the unit vector antiparallel to $T_z \hat{b}_2$ and perpendicular to $T_x \hat{b}_2$ and $T_y \hat{b}_2$. Since \hat{a}_3^{min} is a unit vector, $\|\hat{a}_3^{min}\| = 1$. Again, $\|T_z \hat{b}_2\|^2 = (T_z \hat{b}_2, T_z \hat{b}_2) = (\hat{b}_2, T_z^T T_z \hat{b}_2)$. Since the matrix $T_z^T T_z$ has two equal largest eigenvalues λ_z^{max} , let us consider \hat{b}_2^{max} to be another corresponding unit eigenvector. Then $\|T_z \hat{b}_2\|^2 = (\hat{b}_2, T_z^T T_z \hat{b}_2) = (\hat{b}_2, \lambda_z^{max} \hat{b}_2^{max})$. If \hat{b}_2 is the unit vector along \hat{b}_2^{max} , then $\|T_z \hat{b}_2\|^2 = \lambda_z^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{b}_2 = (0, 0, -\sqrt{\lambda_z^{max}}) \quad (47)$$

(iii) The vector $\hat{b}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned}\hat{b}_3^T \vec{T} \hat{b}_2 &= ((\hat{b}_3, T_x \hat{b}_2), (\hat{b}_3, T_y \hat{b}_2), (\hat{b}_3, T_z \hat{b}_2)) \\ &= (0, 0, -\|\hat{b}_3^{min}\| \|T_y \hat{b}_2\|) \\ &= (0, 0, -\sqrt{\lambda_z^{max}})\end{aligned}\quad (48)$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_z \hat{b}_2$ and perpendicular to $T_x \hat{b}_2$ and $T_y \hat{b}_2$.

(iv) The vector $\hat{b}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned}\hat{b}_3^T \vec{T} \hat{a}_2 &= ((\hat{b}_3, T_x \hat{a}_2), (\hat{b}_3, T_y \hat{a}_2), (\hat{b}_3, T_z \hat{a}_2)) \\ &= (0, 0, -\|\hat{b}_3^{min}\| \|T_y \hat{a}_2\|) \\ &= (0, 0, -\sqrt{\lambda_z^{max}})\end{aligned}\quad (49)$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_z \hat{a}_2$ and perpendicular to $T_x \hat{a}_2$ and $T_y \hat{a}_2$.

From (7),(45),(47),(48),(49), we have

$$\begin{aligned}\langle B_M^{(6)} \rangle_\rho &= \max_{\hat{a}_1, \hat{b}_1} [(\hat{a}_1, (0, 0, \sqrt{\lambda_z^{max}})) \\ &\quad + (\hat{a}_1, (0, 0, \sqrt{\lambda_z^{max}})) + (\hat{b}_1, (0, 0, \sqrt{\lambda_z^{max}})) \\ &\quad + (\hat{b}_1, (0, 0, \sqrt{\lambda_z^{max}}))] \\ &= 2\|\hat{a}_1^{max}\| \|(0, 0, \sqrt{\lambda_z^{max}})\| \\ &\quad + 2\|\hat{b}_1^{max}\| \|(0, 0, \sqrt{\lambda_z^{max}})\| \\ &= 4\sqrt{\lambda_z^{max}}\end{aligned}\quad (50)$$

where \hat{a}_1^{max} and \hat{b}_1^{max} is the unit vector along $(0, 0, \sqrt{\lambda_z^{max}})$. Thus, the maximum expectation value of the Mermin operator with respect to the state ρ is given by

$$\begin{aligned}\langle B_M^{max} \rangle_\rho &= \max\{\langle B_M^{(4)} \rangle_\rho, \langle B_M^{(5)} \rangle_\rho, \langle B_M^{(6)} \rangle_\rho\} \\ &= \max\{4\sqrt{\lambda_x^{max}}, 4\sqrt{\lambda_y^{max}}, 4\sqrt{\lambda_z^{max}}\} \quad (51)\end{aligned}$$

The Mermin inequality is violated if

$$\langle B_M^{max} \rangle_\rho = \max\{4\sqrt{\lambda_x^{max}}, 4\sqrt{\lambda_y^{max}}, 4\sqrt{\lambda_z^{max}}\} > 2 \quad (52)$$

Thus $\max\{\sqrt{\lambda_x^{max}}, \sqrt{\lambda_y^{max}}, \sqrt{\lambda_z^{max}}\} > \frac{1}{2}$. Hence, proved.

Theorem-3: If $T_x^T T_x$ has two equal largest eigenvalues λ_x^{max} and $T_y^T T_y$ and $T_z^T T_z$ has unique largest eigenvalue λ_y^{max} and λ_z^{max} respectively, then Mermin's inequality is violated if

$$\begin{aligned}\langle B_M^{max} \rangle_\rho &= \max\{4\sqrt{\lambda_x^{max}}, 2\sqrt{\lambda_y^{max}}, 2\sqrt{\lambda_z^{max}}\} \\ &> 2 \quad (53)\end{aligned}$$

Proof: In the expression for $\langle B_M \rangle_\rho$ given by Eq. (7), we first simplify the vectors $\hat{a}_3^T \vec{T} \hat{a}_2$, $\hat{b}_3^T \vec{T} \hat{b}_2$, $\hat{b}_3^T \vec{T} \hat{a}_2$, $\hat{a}_3^T \vec{T} \hat{b}_2$.

Case-I: In this case we choose the vectors in such a way that it maximizes the expectation value of the Mermin operator, given by $\langle B_M^{(7)} \rangle_\rho = 4\sqrt{\lambda_x^{max}}$.

(i) The vector $\hat{a}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned}\hat{a}_3^T \vec{T} \hat{a}_2 &= ((\hat{a}_3, T_x \hat{a}_2), (\hat{a}_3, T_y \hat{a}_2), (\hat{a}_3, T_z \hat{a}_2)) \\ &= (\|\hat{a}_3^{max}\| \|T_x \hat{a}_2\|, 0, 0) \quad (54)\end{aligned}$$

where \hat{a}_3^{max} is the unit vector along $T_x \hat{a}_2$ and perpendicular to $T_y \hat{a}_2$ and $T_z \hat{a}_2$. Since \hat{a}_3^{max} is a unit vector, $\|\hat{a}_3^{max}\| = 1$. Again, $\|T_x \hat{a}_2\|^2 = (T_x \hat{a}_2, T_x \hat{a}_2) = (\hat{a}_2, T_x^T T_x \hat{a}_2)$. If λ_x^{max} is the largest eigenvalue of the symmetric matrix $T_x^T T_x$ and \hat{a}_2^{max} is the corresponding unit eigenvector, then $\|T_x \hat{a}_2\|^2 = (\hat{a}_2, T_x^T T_x \hat{a}_2) = (\hat{a}_2, \lambda_x^{max} \hat{a}_2^{max})$. If \hat{a}_2 is the unit vector along \hat{a}_2^{max} , then $\|T_x \hat{a}_2\|^2 = \lambda_x^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{a}_2 = (\sqrt{\lambda_x^{max}}, 0, 0) \quad (55)$$

(ii) The vector $\hat{a}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned}\hat{a}_3^T \vec{T} \hat{b}_2 &= ((\hat{a}_3, T_x \hat{b}_2), (\hat{a}_3, T_y \hat{b}_2), (\hat{a}_3, T_z \hat{b}_2)) \\ &= (-\|\hat{a}_3^{min}\| \|T_x \hat{b}_2\|, 0, 0) \quad (56)\end{aligned}$$

where \hat{a}_3^{min} is the unit vector antiparallel to $T_x \hat{b}_2$ and perpendicular to $T_y \hat{b}_2$ and $T_z \hat{b}_2$. Since \hat{a}_3^{min} is a unit vector, $\|\hat{a}_3^{min}\| = 1$. Again, $\|T_x \hat{b}_2\|^2 = (T_x \hat{b}_2, T_x \hat{b}_2) = (\hat{b}_2, T_x^T T_x \hat{b}_2)$. Since the matrix $T_x^T T_x$ has two equal largest eigenvalues λ_x^{max} , so \hat{b}_2^{max} is another corresponding unit eigenvector. Then $\|T_x \hat{b}_2\|^2 = (\hat{b}_2, T_x^T T_x \hat{b}_2) = (\hat{b}_2, \lambda_x^{max} \hat{b}_2^{max})$. If \hat{b}_2 is the unit vector along \hat{b}_2^{max} , then $\|T_x \hat{b}_2\|^2 = \lambda_x^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{b}_2 = (-\sqrt{\lambda_x^{max}}, 0, 0) \quad (57)$$

(iii) The vector $\hat{b}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned}\hat{b}_3^T \vec{T} \hat{b}_2 &= ((\hat{b}_3, T_x \hat{b}_2), (\hat{b}_3, T_y \hat{b}_2), (\hat{b}_3, T_z \hat{b}_2)) \\ &= (-\|\hat{b}_3^{min}\| \|T_x \hat{b}_2\|, 0, 0) \\ &= (-\sqrt{\lambda_x^{max}}, 0, 0) \quad (58)\end{aligned}$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_x \hat{b}_2$ and perpendicular to $T_y \hat{b}_2$ and $T_z \hat{b}_2$.

(iv) The vector $\hat{b}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned}\hat{b}_3^T \vec{T} \hat{a}_2 &= ((\hat{b}_3, T_x \hat{a}_2), (\hat{b}_3, T_y \hat{a}_2), (\hat{b}_3, T_z \hat{a}_2)) \\ &= (-\|\hat{b}_3^{min}\| \|T_x \hat{a}_2\|, 0, 0) \\ &= (-\sqrt{\lambda_x^{max}}, 0, 0) \quad (59)\end{aligned}$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_x \hat{a}_2$ and perpendicular to $T_y \hat{a}_2$ and $T_z \hat{a}_2$.

From (7), (55), (57), (58), (59), we have

$$\begin{aligned}\langle B_M^{(7)} \rangle_\rho &= \max_{\hat{a}_1, \hat{b}_1} [(\hat{a}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) \\ &+ (\hat{a}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) + (\hat{b}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) \\ &+ (\hat{b}_1, (\sqrt{\lambda_x^{max}}, 0, 0))] \\ &= 2\|\hat{a}_1^{max}\| \|(\sqrt{\lambda_x^{max}}, 0, 0)\| \\ &+ 2\|\hat{b}_1^{max}\| \|(\sqrt{\lambda_x^{max}}, 0, 0)\| \\ &= 4\sqrt{\lambda_x^{max}} \quad (60)\end{aligned}$$

where \hat{a}_1^{max} and \hat{b}_1^{max} is the unit vector along $(\sqrt{\lambda_x^{max}}, 0, 0)$.

Case-II: In this case we choose the vectors in such a way that it maximizes the expectation value of the Mermin operator, given by $\langle B_M^{(8)} \rangle_\rho = 2\sqrt{\lambda_y^{max}}$.

(i) The vector $\hat{a}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned}\hat{a}_3^T \vec{T} \hat{a}_2 &= ((\hat{a}_3, T_x \hat{a}_2), (\hat{a}_3, T_y \hat{a}_2), (\hat{a}_3, T_z \hat{a}_2)) \\ &= (0, \|\hat{a}_3^{max}\| \|T_y \hat{a}_2\|, 0) \quad (61)\end{aligned}$$

where \hat{a}_3^{max} is the unit vector along $T_y \hat{a}_2$ and perpendicular to $T_x \hat{a}_2$ and $T_z \hat{a}_2$. Since \hat{a}_3^{max} is a unit vector, $\|\hat{a}_3^{max}\| = 1$. Again, $\|T_y \hat{a}_2\|^2 = (T_y \hat{a}_2, T_y \hat{a}_2) = (\hat{a}_2, T_y^T T_y \hat{a}_2)$. If λ_y^{max} is the largest eigenvalue of the symmetric matrix $T_y^T T_y$ and \hat{a}_2^{max} is the corresponding unit vector then $\|T_y \hat{a}_2\|^2 = (\hat{a}_2, T_y^T T_y \hat{a}_2) = (\hat{a}_2, \lambda_y^{max} \hat{a}_2^{max})$. If \hat{a}_2 is the unit vector along \hat{a}_2^{max} , then $\|T_y \hat{a}_2\|^2 = \lambda_y^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{a}_2 = (0, \sqrt{\lambda_y^{max}}, 0) \quad (62)$$

(ii) The vector $\hat{a}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned}\hat{a}_3^T \vec{T} \hat{b}_2 &= ((\hat{a}_3, T_x \hat{b}_2), (\hat{a}_3, T_y \hat{b}_2), (\hat{a}_3, T_z \hat{b}_2)) \\ &= (-\|\hat{a}_3^{min}\| \|T_x \hat{b}_2\|, 0, 0) \quad (63)\end{aligned}$$

where \hat{a}_3^{min} is the unit vector antiparallel to $T_x \hat{b}_2$ and perpendicular to $T_y \hat{b}_2$ and $T_z \hat{b}_2$. Since \hat{a}_3^{min} is a unit vector, $\|\hat{a}_3^{min}\| = 1$. Again, $\|T_x \hat{b}_2\|^2 = (T_x \hat{b}_2, T_x \hat{b}_2) =$

$(\hat{b}_2, T_x^T T_x \hat{b}_2)$. If λ_x^{max} is the largest eigenvalue of the symmetric matrix $T_x^T T_x$ and \hat{b}_2^{max} is the corresponding unit vector, then $\|T_x \hat{b}_2\|^2 = (\hat{b}_2, T_x^T T_x \hat{b}_2) = (\hat{b}_2, \lambda_x^{max} \hat{b}_2^{max})$. If \hat{b}_2 is the unit vector along \hat{b}_2^{max} , then $\|T_x \hat{b}_2\|^2 = \lambda_x^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{b}_2 = (-\sqrt{\lambda_x^{max}}, 0, 0) \quad (64)$$

(iii) The vector $\hat{b}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned} \hat{b}_3^T \vec{T} \hat{b}_2 &= ((\hat{b}_3, T_x \hat{b}_2), (\hat{b}_3, T_y \hat{b}_2), (\hat{b}_3, T_z \hat{b}_2)) \\ &= (-\|\hat{b}_3^{min}\| \|T_x \hat{b}_2\|, 0, 0) \\ &= (-\sqrt{\lambda_x^{max}}, 0, 0) \end{aligned} \quad (65)$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_x \hat{b}_2$ and perpendicular to $T_y \hat{b}_2$ and $T_z \hat{b}_2$. Since \hat{b}_3^{min} is a unit vector, $\|\hat{b}_3^{min}\| = 1$.

(iv) The vector $\hat{b}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned} \hat{b}_3^T \vec{T} \hat{a}_2 &= ((\hat{b}_3, T_x \hat{a}_2), (\hat{b}_3, T_y \hat{a}_2), (\hat{b}_3, T_z \hat{a}_2)) \\ &= (0, \|\hat{b}_3^{max}\| \|T_y \hat{a}_2\|, 0) = (0, \sqrt{\lambda_y^{max}}, 0) \end{aligned} \quad (66)$$

where \hat{b}_3^{max} is the unit vector along $T_y \hat{a}_2$ and perpendicular to $T_x \hat{a}_2$ and $T_z \hat{a}_2$.

From (7),(62),(64),(65),(66), we have

$$\begin{aligned} \langle B_M^{(8)} \rangle_\rho &= \max_{\hat{a}_1, \hat{b}_1} [(\hat{a}_1, (0, \sqrt{\lambda_y^{max}}, 0)) \\ &+ (\hat{a}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) - (\hat{b}_1, (0, \sqrt{\lambda_y^{max}}, 0)) \\ &+ (\hat{b}_1, (\sqrt{\lambda_x^{max}}, 0, 0))] \\ &= \|\hat{a}_1^{max}\| \|(0, \sqrt{\lambda_y^{max}}, 0)\| \\ &+ \|\hat{b}_1^{max}\| \|(0, \sqrt{\lambda_y^{max}}, 0)\| \\ &= 2\sqrt{\lambda_y^{max}} \end{aligned} \quad (67)$$

\hat{a}_1^{max} is the unit vector parallel to $(0, \sqrt{\lambda_y^{max}}, 0)$ and perpendicular to $(\sqrt{\lambda_x^{max}}, 0, 0)$; \hat{b}_1^{max} is the unit vectors antiparallel to $(0, \sqrt{\lambda_y^{max}}, 0)$ and perpendicular to $(\sqrt{\lambda_x^{max}}, 0, 0)$.

Case-III: In this case we choose the vectors in such a way that it maximizes the expectation value of the Mermin operator, given by $\langle B_M^{(9)} \rangle_\rho = 2\sqrt{\lambda_z^{max}}$.

(i) The vector $\hat{a}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned} \hat{a}_3^T \vec{T} \hat{a}_2 &= ((\hat{a}_3, T_x \hat{a}_2), (\hat{a}_3, T_y \hat{a}_2), (\hat{a}_3, T_z \hat{a}_2)) \\ &= (0, 0, \|\hat{a}_3^{max}\| \|T_z \hat{a}_2\|) \end{aligned} \quad (68)$$

where \hat{a}_3^{max} is the unit vector along $T_z \hat{a}_2$ and perpendicular to $T_x \hat{a}_2$ and $T_y \hat{a}_2$. Since \hat{a}_3^{max} is a unit vector, $\|\hat{a}_3^{max}\| = 1$. Again, $\|T_z \hat{a}_2\|^2 = (T_z \hat{a}_2, T_z \hat{a}_2) = (\hat{a}_2, T_z^T T_z \hat{a}_2)$. If λ_z^{max} is the largest eigenvalue of the symmetric matrix $T_z^T T_z$ and \hat{a}_2^{max} is the corresponding unit vector then $\|T_z \hat{a}_2\|^2 =$

$(\hat{a}_2, T_z^T T_z \hat{a}_2) = (\hat{a}_2, \lambda_z^{max} \hat{a}_2^{max})$. If \hat{a}_2 is the unit vector along \hat{a}_2^{max} , then $\|T_z \hat{a}_2\|^2 = \lambda_z^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{a}_2 = (0, 0, \sqrt{\lambda_z^{max}}) \quad (69)$$

(ii) The vector $\hat{a}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned} \hat{a}_3^T \vec{T} \hat{b}_2 &= ((\hat{a}_3, T_x \hat{b}_2), (\hat{a}_3, T_y \hat{b}_2), (\hat{a}_3, T_z \hat{b}_2)) \\ &= (-\|\hat{a}_3^{min}\| \|T_x \hat{b}_2\|, 0, 0) \end{aligned} \quad (70)$$

where \hat{a}_3^{min} is the unit vector antiparallel to $T_x \hat{b}_2$ and perpendicular to $T_y \hat{b}_2$ and $T_z \hat{b}_2$. Since \hat{a}_3^{min} is a unit vector, $\|\hat{a}_3^{min}\| = 1$. Again, $\|T_x \hat{b}_2\|^2 = (T_x \hat{b}_2, T_x \hat{b}_2) = (\hat{b}_2, T_x^T T_x \hat{b}_2)$. If λ_x^{max} is the largest eigenvalue of the symmetric matrix $T_x^T T_x$ and \hat{b}_2^{max} is the corresponding unit vector then $\|T_x \hat{b}_2\|^2 = (\hat{b}_2, T_x^T T_x \hat{b}_2) = (\hat{b}_2, \lambda_x^{max} \hat{b}_2^{max})$. If \hat{b}_2 is the unit vector along \hat{b}_2^{max} then $\|T_x \hat{b}_2\|^2 = \lambda_x^{max}$. Thus,

$$\hat{a}_3^T \vec{T} \hat{b}_2 = (-\sqrt{\lambda_x^{max}}, 0, 0) \quad (71)$$

(iii) The vector $\hat{b}_3^T \vec{T} \hat{b}_2$ can be simplified as

$$\begin{aligned} \hat{b}_3^T \vec{T} \hat{b}_2 &= ((\hat{b}_3, T_x \hat{b}_2), (\hat{b}_3, T_y \hat{b}_2), (\hat{b}_3, T_z \hat{b}_2)) \\ &= (-\|\hat{b}_3^{min}\| \|T_x \hat{b}_2\|, 0, 0) \\ &= (-\sqrt{\lambda_x^{max}}, 0, 0) \end{aligned} \quad (72)$$

where \hat{b}_3^{min} is the unit vector antiparallel to $T_x \hat{b}_2$ and perpendicular to $T_y \hat{b}_2$ and $T_z \hat{b}_2$. Since \hat{b}_3^{min} is a unit vector, $\|\hat{b}_3^{min}\| = 1$.

(iv) The vector $\hat{b}_3^T \vec{T} \hat{a}_2$ can be simplified as

$$\begin{aligned} \hat{b}_3^T \vec{T} \hat{a}_2 &= ((\hat{b}_3, T_x \hat{a}_2), (\hat{b}_3, T_y \hat{a}_2), (\hat{b}_3, T_z \hat{a}_2)) \\ &= (0, 0, \|\hat{b}_3^{max}\| \|T_z \hat{a}_2\|) = (0, 0, \sqrt{\lambda_z^{max}}) \end{aligned} \quad (73)$$

where \hat{b}_3^{max} is the unit vector along $T_z \hat{a}_2$ and perpendicular to $T_x \hat{a}_2$ and $T_y \hat{a}_2$.

From (7),(69),(71),(72),(73), we have

$$\begin{aligned} \langle B_M^{(9)} \rangle_\rho &= \max_{\hat{a}_1, \hat{b}_1} [(\hat{a}_1, (0, 0, \sqrt{\lambda_z^{max}})) \\ &+ (\hat{a}_1, (\sqrt{\lambda_x^{max}}, 0, 0)) - (\hat{b}_1, (0, 0, \sqrt{\lambda_z^{max}})) \\ &+ (\hat{b}_1, (\sqrt{\lambda_x^{max}}, 0, 0))] \\ &= \|\hat{a}_1^{max}\| \|(0, 0, \sqrt{\lambda_z^{max}})\| \\ &+ \|\hat{b}_1^{max}\| \|(0, 0, \sqrt{\lambda_z^{max}})\| \\ &= 2\sqrt{\lambda_z^{max}} \end{aligned} \quad (74)$$

\hat{a}_1^{max} is the unit vector parallel to $(0, 0, \sqrt{\lambda_z^{max}})$ and perpendicular to $(\sqrt{\lambda_x^{max}}, 0, 0)$; \hat{b}_1^{max} is the unit vectors antiparallel to $(0, 0, \sqrt{\lambda_z^{max}})$ and perpendicular to $(\sqrt{\lambda_x^{max}}, 0, 0)$. Thus, the maximum expectation value of the Mermin operator with respect to the state ρ is given by

$$\begin{aligned} \langle B_M^{max} \rangle_\rho &= \max\{\langle B_M^{(7)} \rangle_\rho, \langle B_M^{(8)} \rangle_\rho, \langle B_M^{(9)} \rangle_\rho\} \\ &= \max\{4\sqrt{\lambda_x^{max}}, 2\sqrt{\lambda_y^{max}}, 2\sqrt{\lambda_z^{max}}\} \end{aligned} \quad (75)$$

Mermin inequality is violated if

$$\langle B_M^{max} \rangle_\rho = \max\{4\sqrt{\lambda_x^{max}}, 2\sqrt{\lambda_y^{max}}, 2\sqrt{\lambda_z^{max}}\} > 2 \quad (76)$$

Thus $\max\{2\sqrt{\lambda_x^{max}}, \sqrt{\lambda_y^{max}}, \sqrt{\lambda_z^{max}}\} > 1$. Hence, proved.

Corollary-1: If $T_y^T T_y$ has two equal largest eigenvalues λ_y^{max} and $T_x^T T_x$ and $T_z^T T_z$ have unique largest eigenvalues λ_x^{max} and λ_z^{max} respectively, then Mermin's inequality is violated if

$$\begin{aligned} \langle B_M^{max} \rangle_\rho &= \max\{2\sqrt{\lambda_x^{max}}, 4\sqrt{\lambda_y^{max}}, 2\sqrt{\lambda_z^{max}}\} \\ &> 2 \end{aligned} \quad (77)$$

Corollary-2: If $T_z^T T_z$ has two equal largest eigenvalues λ_z^{max} , and $T_x^T T_x$ and $T_y^T T_y$ have unique largest eigenvalue λ_x^{max} and λ_y^{max} respectively, then Mermin's inequality is violated if

$$\begin{aligned} \langle B_M^{max} \rangle_\rho &= \max\{2\sqrt{\lambda_x^{max}}, 2\sqrt{\lambda_y^{max}}, 4\sqrt{\lambda_z^{max}}\} \\ &> 2 \end{aligned} \quad (78)$$

Corollary-3: If $T_x^T T_x$ and $T_y^T T_y$ have two equal largest eigenvalues λ_x^{max} and λ_y^{max} respectively, and $T_z^T T_z$ has unique largest eigenvalue λ_z^{max} , then Mermin's inequality is violated if

$$\begin{aligned} \langle B_M^{max} \rangle_\rho &= \max\{4\sqrt{\lambda_x^{max}}, 4\sqrt{\lambda_y^{max}}, 2\sqrt{\lambda_z^{max}}\} \\ &> 2 \end{aligned} \quad (79)$$

Corollary-4: If $T_x^T T_x$ and $T_z^T T_z$ have two equal largest eigenvalue λ_x^{max} and λ_z^{max} , respectively and $T_y^T T_y$ has unique largest eigenvalue λ_y^{max} , then Mermin's inequality is violated if

$$\begin{aligned} \langle B_M^{max} \rangle_\rho &= \max\{4\sqrt{\lambda_x^{max}}, 2\sqrt{\lambda_y^{max}}, 4\sqrt{\lambda_z^{max}}\} \\ &> 2 \end{aligned} \quad (80)$$

Corollary-5: If $T_y^T T_y$ and $T_z^T T_z$ have two equal largest eigenvalue λ_y^{max} and λ_z^{max} respectively, and $T_x^T T_x$ has unique largest eigenvalue λ_x^{max} , then Mermin's inequality is violated if

$$\begin{aligned} \langle B_M^{max} \rangle_\rho &= \max\{2\sqrt{\lambda_x^{max}}, 4\sqrt{\lambda_y^{max}}, 4\sqrt{\lambda_z^{max}}\} \\ &> 2 \end{aligned} \quad (81)$$

III. EXAMPLES

Example-1: The generalized GHZ state can be written in terms of Pauli matrices as

$$\begin{aligned} \rho_{GGHZ} &= \frac{1}{8}[I \otimes I \otimes I + I \otimes \sigma_z \otimes \sigma_z + \sigma_z \otimes I \otimes \sigma_z \\ &+ \sigma_z \otimes \sigma_z \otimes I + (\alpha^2 - \beta^2)(\sigma_z \otimes I \otimes I \\ &+ I \otimes \sigma_z \otimes I + I \otimes I \otimes \sigma_z) + 2\alpha\beta(\sigma_x \otimes \sigma_x \otimes \sigma_x \\ &- \sigma_x \otimes \sigma_y \otimes \sigma_y - \sigma_y \otimes \sigma_x \otimes \sigma_y \\ &- \sigma_y \otimes \sigma_y \otimes \sigma_x)], \quad \alpha^2 + \beta^2 = 1 \end{aligned} \quad (82)$$

The matrices $T_x^T T_x, T_y^T T_y$ are given by

$$T_x^T T_x = T_y^T T_y = \begin{pmatrix} 4\alpha^2\beta^2 & 0 & 0 \\ 0 & 4\alpha^2\beta^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (83)$$

The matrix $T_z^T T_z$ is a zero matrix. The largest eigenvalues of the matrices $T_x^T T_x, T_y^T T_y$ are given by

$$\begin{aligned} \lambda_x^{max} &= 4\alpha^2\beta^2 \\ \lambda_y^{max} &= 4\alpha^2\beta^2 \end{aligned} \quad (84)$$

The maximum expectation value of the Mermin operator with respect to the state ρ_{GGHZ} is given by

$$\langle B_M^{max} \rangle_{\rho_{GGHZ}} = 8\alpha\beta \quad (85)$$

Therefore, the generalized GHZ state violates Mermin's inequality if

$$2\alpha\beta > \frac{1}{2} \quad (86)$$

The same result has been found numerically by Scarani and Gisin [16].

Example-2: Let us consider a pure state which is a coherent superposition of the W -state and a separable state $|000\rangle$. The superposed state can be expressed as

$$|\Psi\rangle_{W,S} = \sqrt{1-p}|W\rangle + \sqrt{p}|000\rangle, \quad 0 \leq p \leq 1 \quad (87)$$

where $|W\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle)$. In this case the symmetric matrices $T_x^T T_x, T_y^T T_y, T_z^T T_z$ take the form

$$\begin{aligned} T_x^T T_x &= \begin{pmatrix} \frac{4}{9}(1-p)^2 & 0 & \frac{4}{3\sqrt{3}}\sqrt{p}(1-p)^{\frac{3}{2}} \\ 0 & 0 & 0 \\ \frac{4}{3\sqrt{3}}\sqrt{p}(1-p)^{\frac{3}{2}} & 0 & \frac{4}{9}(1-p)(1+2p) \end{pmatrix} \\ T_y^T T_y &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{4}{9}(1-p)^2 & 0 \\ 0 & 0 & \frac{4}{9}(1-p)^2 \end{pmatrix} \\ T_z^T T_z &= \begin{pmatrix} \frac{4}{9}(1-p)(1+2p) & 0 & f \\ 0 & \frac{4}{9}(1-p)^2 & 0 \\ f & 0 & g \end{pmatrix} \end{aligned} \quad (88)$$

where $f = \frac{4}{3\sqrt{3}}\sqrt{p}(1-p)^{\frac{3}{2}} + \frac{2}{\sqrt{3}}\sqrt{p}\sqrt{1-p}(2p-1)$ and $g = \frac{4}{3}p(1-p) + (2p-1)^2$. The largest eigenvalues of the matrices $T_x^T T_x, T_y^T T_y, T_z^T T_z$ are given by

$$\begin{aligned} \lambda_x^{max} &= (1-p)\left(\frac{4}{9} + \frac{2}{9}p + \frac{2}{9}\sqrt{12p-3p^2}\right) \\ \lambda_y^{max} &= \frac{4}{9}(1-p)^2 \\ \lambda_z^{max} &= \frac{1}{18}\sqrt{256p^4 - 640p^3 + 672p^2 - 232p + 25} \\ &+ \frac{13}{18} + \frac{8}{9}p^2 - \frac{10}{9}p \end{aligned} \quad (89)$$

The maximum expectation value of the Mermin operator with respect to the state $|\Psi\rangle_{W,S}$ is given by

$$\begin{aligned}\langle B_M^{max} \rangle_{|\Psi\rangle_{W,S}|\Psi\rangle} &= 4\sqrt{\lambda_y^{max}} \quad 0 \leq p \leq 0.43 \\ \langle B_M^{max} \rangle_{|\Psi\rangle_{W,S}|\Psi\rangle} &= 2\sqrt{\lambda_x^{max}}, \quad 0.43 \leq p \leq 0.45 \\ \langle B_M^{max} \rangle_{|\Psi\rangle_{W,S}|\Psi\rangle} &= 2\sqrt{\lambda_z^{max}}, \quad 0.45 \leq p \leq 1\end{aligned}\quad (90)$$

It can be easily seen from figs.1(a), fig.1(b), fig.1(c) that the state $|\Psi\rangle_{W,S}$ violates Mermin's inequality when $0 \leq p \leq 0.25$. This result was obtained in [19].

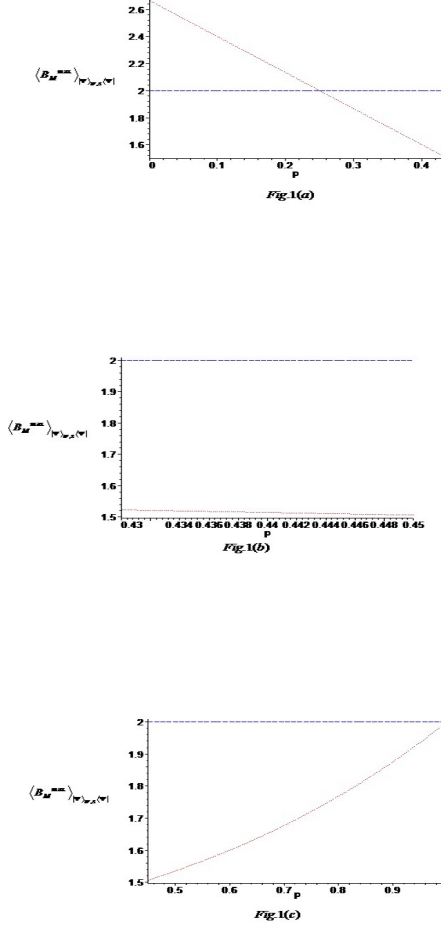


FIG. 1: Violation of the Mermin inequality versus the state parameter p for the pure state given by Eq.(87)

Example-3: Let us consider a mixed state ϱ which is described by the density operator

$$\varrho = p|\psi\rangle_{GHZ}\langle\psi| + (1-p)|\psi\rangle_W\langle\psi| \quad (91)$$

where $|\psi\rangle_{GHZ} = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ and $|\psi\rangle_W = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle)$. Our task is to find out the range of the parameter p for which ϱ violates the Mermin inequality. Hence, we have to calculate the largest eigenvalues of the symmetric

matrices $T_x^T T_x, T_y^T T_y, T_z^T T_z$. Since in this case the matrices $T_y^T T_y, T_z^T T_z$ have two equal largest eigenvalues, and $T_x^T T_x$ has a unique largest eigenvalue, one has

$$\langle B_M^{max} \rangle_{\varrho} = \max\{2\sqrt{\lambda_x^{max}}, 4\sqrt{\lambda_y^{max}}, 4\sqrt{\lambda_z^{max}}\} \quad (92)$$

where $\lambda_x^{max} = \frac{4}{9} - \frac{8}{9}p + \frac{17}{18}p^2 + \frac{1}{6}\sqrt{25p^4 - 32p^3 + 16p^2}$, $\lambda_y^{max} = \frac{4}{9} - \frac{8}{9}p + \frac{13}{9}p^2$, and $\lambda_z^{max} = (1-p)^2$. It follows from Eq.(92) that

$$\begin{aligned}\langle B_M^{max} \rangle_{\varrho} &= 4(1-p), \quad 0 \leq p \leq 0.43 \\ &= 4\sqrt{\frac{4}{9} - \frac{8}{9}p + \frac{13}{9}p^2}, \quad 0.43 \leq p \leq 1\end{aligned}\quad (93)$$

Fig.2(a) and Fig.2(b) clearly show that the mixed state ϱ violates Mermin's inequality for all values of the parameter p , i.e., $0 \leq p \leq 1$.

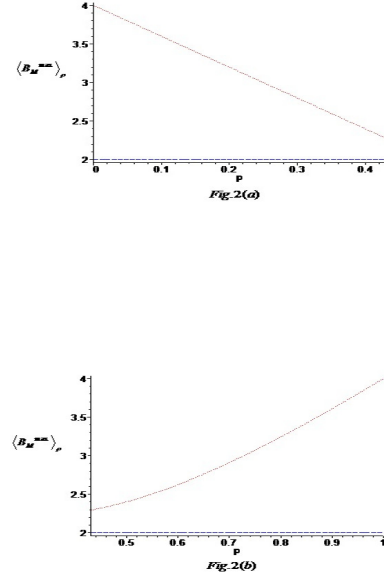


FIG. 2: Violation of the Mermin inequality versus the state parameter p for the mixed state given by Eq.(91)

IV. CONCLUSIONS

In this work we have studied Mermin's inequality for three qubit states, the violation of which predicts the existence of quantum correlations between the outcomes of the distant measurements on three qubit systems. Prior to this work there did not exist in the literature any closed form expression that gives the maximal violation of the Mermin inequality. Motivated by the analogous criterion for two qubit systems [15], we have here presented some analytical formulae in terms of eigenvalues of symmetric matrices, that provide conditions for

violating the Mermin inequality by both pure and mixed arbitrary three qubit states. Our results are useful in obtaining the violation of Mermin's inequality because using them one does not need to perform optimization procedures over spin measurements in all possible directions. We have illustrated our

results with a few examples of pure and mixed states, confirming the range of violation of the Mermin inequality obtained in earlier works [17, 19].

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